Path-integral solution for a Mie-type potential

Ş. Erkoç and R. Sever
Department of Physics, Middle East Technical University, Ankara, Turkey
(Received 14 June 1984)

A path-integral solution for a Mie-type potential is obtained. The exact eigensolutions for a special case of the potential are calculated.

I. INTRODUCTION

The path-integral formulation of Feynman[1] offers an alternative approach for solving dynamical problems in quantum mechanics. A great interest has recently been devoted to the application of this technique to the exactly solvable problems by the Schrödinger equation.[2] To apply this technique one usually follows the point canonical transformation and a change of time parameter to reduce the problem to a proper form that has an exact solution.

Recently the H-atom[3] and one-dimensional Morse-potential Green's function[4] have been calculated with the path integral, by converting them to a four-dimensional harmonic oscillator, and a one-dimensional harmonic oscillator with an additional potential barrier, respectively.

In recent years Mie-type potentials[5] have been used to study the dynamical properties of solids,[6] and are given by

$$V(x)=\epsilon\left[\frac{k}{l-k}\left[\frac{\sigma}{x}\right]^{l}-\frac{l}{l-k}\left[\frac{\sigma}{x}\right]^{k}\right], \tag{1}$$

where ϵ is the interaction energy between two atoms in a solid at $x=\sigma$, and $l>k$ is always satisfied.

In the present study we solve the path integral for the one-dimensional Mie potential with $l=2k$ combination. Choosing the special case $k=1$, corresponding to a Coulombic-type potential with an additional centrifugal potential barrier, we test the validity of our transformations by comparing the results with the known exact eigensolutions of a Coulombic potential.

II. PATH INTEGRAL FOR $V(x)$

The probability amplitude for a particle of mass m traveling from a position x_a at time $t_a=0$ to x_b at time $t_b=T$ in a Mie-type potential with $l=2k$,

$$V(x)=V_0\left[\frac{1}{2k}\left[\frac{\sigma}{x}\right]^{2k}-\frac{1}{k}\left[\frac{\sigma}{x}\right]^{k}\right], \quad V_0=2\epsilon k \tag{2}$$

can be written as the phase-space path integral in Cartesian coordinates:[7]

$$K(x_b,T;x_a,0)=\int\frac{Dx\,Dp}{2\pi}\exp\left[\frac{i}{\hbar}\int_0^T dt\left[p\dot{x}-\frac{p^2}{2m}-V(x)\right]\right] \tag{3}$$

which is understood as the limiting case of its time-graded form

$$K(x_b,T;x_a,0)=\lim_{\substack{n\to\infty\\ \epsilon\to 0}}\int\prod_{i=1}^{n}dx_i\prod_{i=1}^{n+1}\frac{dp_i}{2\pi}\exp\left\{\frac{i}{\hbar}\sum_{i=1}^{n+1}\left[p_i(x_i-x_{i-1})-\epsilon\left[\frac{p_i^2}{2m}-V(x_i)\right]\right]\right\}, \tag{4}$$

where $\epsilon=t_i-t_{i-1}$, $(n+1)\epsilon=t_b-t_a=T$, and $x_0=x_a$, $x_{n+1}=x_b$.

We define a new coordinate $Q\in(0,\infty)$ with the point canonical transformations

$$x=\sigma Q^{1/k}, \quad p=\left[\frac{k}{\sigma}Q^{1-1/k}\right]P \tag{5}$$

generated from the function

$$F_2(x,P)=\left[\frac{x}{\sigma}\right]^k P.$$

After evaluating the Jacobian at the point b, the path integral in Eq. (3) takes the form

$$K(x_b,T;x_a,0)=\left[\frac{k}{\sigma}Q_b^{1-1/k}\right]\int\frac{DQ\,DP}{2\pi}\exp\left\{\frac{i}{\hbar}\int_0^T dt\left[P\dot{Q}-\frac{1}{2m}\left[\frac{k}{\sigma}\right]^2 Q^{2(1-1/k)}P^2-\frac{V_0}{k}\left[\frac{1}{2}\frac{1}{Q^2}-\frac{1}{Q}\right]\right]\right\}. \tag{6}$$

Introducing a new time variable s by

$$dt=\left[\frac{\sigma}{k}Q^{1/k-1}\right]^2 ds \tag{7}$$

we eliminate the factor of the kinetic energy term. Similar transformations on the time parameter have been used previously.[3,4] With the constraint

$$T=\left[\frac{\sigma}{k}\right]^2 \int^S ds(Q(s))^{2(1/k-1)}\ , \quad S=s_b-s_a \tag{8}$$

Eq. (6) may be written as

$$K(x_b,T;x_a,0)=\int \left[\frac{k}{\sigma}Q_b{}^{1-1/k}\right]\left[\frac{\sigma}{k}Q_b{}^{1/k-1}\right]^2 \times\int_0^\infty dS\delta\left[T-\int_0^S ds\left[\frac{\sigma}{k}\right]^2(Q(s))^{2(1/k-1)}\right]\frac{DQ(s)DP(s)}{2\pi} \times\exp\left\{\frac{i}{\hbar}\int_0^S ds\left[\frac{\sigma}{k}Q^{1/k-1}\right]^2\left[PQ'\left[\frac{ds}{dt}\right]-\left[\frac{k}{\sigma}Q^{1-1/k}\right]^2\frac{p^2}{2m}-\frac{V_0}{k}\left[\frac{1}{2}\frac{1}{Q^2}-\frac{1}{Q}\right]\right]\right\}, \tag{9}$$

where the prime denotes the derivative with respect to s. Introducing the Fourier representation of the δ function, the path integral takes the form

$$K(x_b,T;x_a,0)=\left[\frac{\sigma}{k}\right]\int_{-\infty}^{+\infty}\frac{dE}{2\pi}e^{iEt}\int_0^\infty dS\int(Q_b{}^{1/k-1})\frac{DQ\,DP}{2\pi} \times\exp\left\{\frac{i}{\hbar}\int_0^S ds\left[PQ'-\frac{P^2}{2m}-\frac{V_0}{k}\left[\frac{\sigma}{k}\right]^2(\tfrac{1}{2}Q^{2/k-4}-Q^{2/k-3})-\hbar E\left[\frac{\sigma}{k}\right]^2Q^{2/k-2}\right]\right\}. \tag{10}$$

The end points a and b should have equal contributions to the Jacobian in order to have a symmetric Jacobian. This is possible by rewriting the factor $Q_b{}^{1/k-1}$ as

$$Q_b{}^{1/k-1}=(Q_b{}^{1/k-1}Q_a{}^{1/k-1})^{1/2}\exp[\tfrac{1}{2}\ln(Q_b{}^{1/k-1}/Q_a{}^{1/k-1})]$$
$$=(Q_b{}^{1/k-1}Q_a{}^{1/k-1})^{1/2}\exp\left[\frac{i}{\hbar}\int_0^S ds\frac{i\hbar}{2}\left[1-\frac{1}{k}\right]\frac{Q'}{Q}\right]. \tag{11}$$

The path integral given in Eq. (4) would also be expressed by starting the time division of the momentum variables at $i=0$ and ending at $i=n$. In this case we would have a Jacobian $Q_a{}^{1/k-1}$. Following the same procedure to symmetrize the Jacobian we then get

$$Q_a{}^{1/k-1}=(Q_b{}^{1/k-1}Q_a{}^{1/k-1})^{1/2}\exp\left[\frac{i}{\hbar}\int_0^S ds\frac{i\hbar}{2}\left[\frac{1}{k}-1\right]\frac{Q'}{Q}\right]. \tag{12}$$

The contributions of the symmetrized Jacobians, Eqs. (11) and (12), to the integrand of the path integral, Eq. (10), are the same in magnitude, but opposite in sign. If we then use the midpoint method by taking the arithmetic mean of the integrands, we obtain

$$\bar{K}(x_b,T;x_a,0)=\left[\frac{\sigma}{k}\right]\int_{-\infty}^{+\infty}\frac{dE}{2\pi}e^{iET}\int_0^\infty dS\int(Q_b{}^{1/k-1}Q_a^{1/k-1})^{1/2}\frac{DQ\,DP}{2\pi} \times\exp\left\{\frac{i}{\hbar}\int_0^S ds\left[PQ'-\frac{P^2}{2m}-\frac{V_0}{k}\left[\frac{\sigma}{k}\right]^2(\tfrac{1}{2}Q^{2/k-4}-Q^{2/k-3})-\hbar E\left[\frac{\sigma}{k}\right]^2Q^{2/k-2}\right]\right\}, \tag{13}$$

Setting $k=1$, Eq. (13) becomes

$$\bar{K}(x_b,T;x_a,0)=\sigma\int_{-\infty}^{+\infty}\frac{dE}{2\pi}e^{iET}\int_0^\infty dS\int\frac{DQ\,DP}{2\pi}\exp\left\{\frac{i}{\hbar}\int_0^S ds\left[PQ'-\frac{P^2}{2m}-V_o\sigma^2\left[\frac{1}{2Q^2}-\frac{1}{Q}\right]-\sigma^2\hbar E\right]\right\}, \tag{14}$$

or equivalently, as

$$\bar{K}(x_b,T;x_a,0)=\sigma\int_{-\infty}^{+\infty}\frac{dE}{2\pi}e^{iET}\int_0^{\infty}dS\,\mathrm{K}(Q_b,S;Q_a,0)\ , \tag{15}$$

where the kernel is

$$\mathrm{K}(Q_b,S;Q_a,0)=\int\frac{DQ\,DP}{2\pi}\exp\left\{\frac{i}{\hbar}\int_0^S ds\left[PQ'-\frac{P^2}{2m}-V_0\sigma^2\left[\frac{1}{2Q^2}-\frac{1}{Q}\right]-\sigma^2\hbar E\right]\right\}\ , \tag{16}$$

its effective Hamiltonian is

$$H_{\text{eff}}=\frac{P^2}{2m}+\sigma^2V_0\left[\frac{1}{2Q^2}-\frac{1}{Q}\right]+\sigma^2\hbar E\ . \tag{17}$$

The path integral can also be expressed in terms of the eigensolutions of the system described by

$$\bar{K}(x_b,T;x_a,0)=\sum_n e^{-iE_nT}\Phi_n(x_b)\Phi_n^*(x_a)\ . \tag{18}$$

Let us define a new effective Hamiltonian as

$$H'_{\text{eff}}=H_{\text{eff}}-\sigma^2\hbar E \tag{19a}$$

$$=\frac{P^2}{2m}+\sigma^2V_0\left[\frac{1}{2Q^2}-\frac{1}{Q}\right] \tag{19b}$$

$$=\frac{P^2}{2m}+\frac{A}{Q^2}-\frac{B}{Q}\ , \tag{19c}$$

where $A=\frac{1}{2}\sigma^2V_0$, and $B=\sigma^2V_0$. The eigenvalues of the H'_{eff} are given by[8]

$$\epsilon'_n=-\frac{2B^2m}{\hbar^2}\left\{2(n-s-1)+1+\left[(2l+1)^2+\frac{8mA}{\hbar}\right]^{1/2}\right\}^{-2} \tag{20}$$

for the eigenfunctions

$$\Psi_n(Q)=N\rho^se^{-\rho/2}F(-n+s+1,2(s+1),\rho)\ , \tag{21}$$

where

$$\rho=2\left[\frac{-2mE}{\hbar^2}\right]^{1/2}Q\ , \tag{22a}$$

$$s=\frac{1}{2}\left[-1+\left[(2l+1)^2+\frac{8mA}{\hbar^2}\right]^{1/2}\right]>0\ , \tag{22b}$$

$$n=B\left[\frac{-m}{2E\hbar^2}\right]^{1/2}\ , \tag{22c}$$

$$N=\frac{1}{(2s+1)!}\left[\frac{(n+s)!}{2n(n-s-1)!}\right]^{1/2}\ , \tag{22d}$$

and F is the confluent hypergeometric function.

The kernel, Eq. (16), may be expanded in terms of the eigensolutions of the effective Hamiltonian, H_{eff},

$$\mathrm{K}(Q_b,S;Q_a,0)=\sum_n e^{-(i/\hbar)\epsilon_nS}\psi_n(Q_b)\psi_n^*(Q_a)\ . \tag{23}$$

The eigenvalues, ϵ_n, may be obtained from

$$\epsilon_n=\epsilon'_n+\sigma^2\hbar E\ . \tag{24}$$

Inserting Eq. (23) into Eq. (15), the path integral takes the form

$$\bar{K}(x_b,T;x_a,0)=\sigma\int_{-\infty}^{+\infty}\frac{dE}{2\pi}e^{iET}\int_0^{\infty}dS\sum_n e^{-(i/\hbar)\epsilon_nS}\psi_n(Q_b)\psi_n^*(Q_a)\ , \tag{25}$$

integrating over S we obtain

$$\bar{K}(x_b,T;x_a,0)=\sum_n\int_{-\infty}^{+\infty}\frac{dE}{2\pi}\frac{i}{\sigma}\frac{e^{iET}}{(E+\epsilon'_n/\sigma^2\hbar)}\psi_n(Q_b)\psi_n^*(Q_a)\ , \tag{26}$$

and finally integrating over E we get

$$\bar{K}(x_b,T;x_a,0)=\sum_n e^{-i(E'_n/\sigma^2\hbar)T}\left[\frac{1}{\sqrt{\sigma}}\psi_n(Q_b)\right]\left[\frac{1}{\sqrt{\sigma}}\psi_n(Q_a)\right]^* \tag{27a}$$

or

$$=\sum_n e^{-iE_nT}\Phi_n(Q_b)\Phi_n^*(Q_a)\ , \tag{27b}$$

where

$$E_n=\frac{E'_n}{\sigma^2\hbar}=-\frac{2m}{\hbar^2}\frac{\sigma^2V_0{}^2}{\hbar}\left\{2(n-s-1)+1+\left[(2l+1)^2+\frac{2m}{\hbar^2}2\sigma^2V_0\right]^{1/2}\right\}^{-2} \tag{28}$$

and

$$\Phi_n(Q)=\frac{1}{(2s+1)!}\left[\frac{(n+s)!}{2n(n-s-1)!}\right]^{1/2}\rho^se^{-\rho/2}\times F(-n+s+1,2(s+1),\rho)\ . \tag{29}$$

s can be eliminated in Eq. (28) by using Eq. (22b), hence the eigenvalues can be reduced to the following simple form:

$$E_n = -\frac{2m}{\hbar^2}\frac{\sigma^4 V_0{}^2}{4n^2}\ , \quad n=1,2,3,\ldots \ . \tag{30}$$

As a result the path integral takes the final form

$$\bar{K}(x_b,T;x_a,0)=\sum_{n=1}^{\infty}\exp\left[i\left[\frac{2m}{\hbar^2}\frac{\sigma^4 V_0{}^2}{4n^2}\right]T\right] \times\frac{(n+s)!}{2n(n-s-1)!}\frac{\rho_b^s\rho_a^s}{[(2s+1)]^2} \times e^{-(\rho_b+\rho_a)/2}F(-n+s+1,2(s+1),\rho_b) \times F(-n+s+1,2(s+1),\rho_a)\ . \tag{31}$$

III. CONCLUSIONS

In this work we have studied the path-integral solution for a Mie-type potential. The point canonical transformations were generated from a second-type function of the form $F_2(x,P)$. Considering the special case of the Mie potential with $l=2k$ and for $k=1$, the problem was reduced to a Coulombic potential with an additional centrifugal potential barrier $1/Q^2$. The exact eigensolutions for this particular case have been obtained, which are similar to the hydrogenic solutions.

ACKNOWLEDGMENTS

This research was partially supported by the Scientific and Technical Research Council of Turkey.

[1]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[2]L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).
[3]I. H. Duru and H. Kleinert, Phys. Lett. **84B**, 185 (1975); Fortschr. Phys. **30**, 401 (1982).
[4]I. H. Duru, Phys. Rev. D **28**, 2689 (1983); N. K. Pak and I. Sökmen, Phys. Lett. **100A**, 327 (1984).
[5]G. Mie, Ann. Phys. (Leipzig) **11**, 657 (1903).
[6]See, for example, *Rare Gas Solids,* edited by M. L. Klein and J. A. Venables (Academic, London, 1976), Vol. 1.
[7]H. Davies, Proc. Cambridge Philos. Soc. **59**, 147 (1963).
[8]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics (Nonrelativistic Theory),* third ed. (Pergamon, New York, 1977), p. 127.